ABSTRACT CODE

Fermi surface studies of UGa_3 – positron annihilation experiment and ab-initio calculations

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UGa_3 is a moderate heavy fermion system ordering in a simple magnetic structure with U moments aligned antiferromagnetically in adjacent (111) ferromagnetic planes. The Sommerfeld coefficient and Neel temperature are 52 mJ/K^2 mol and 67 K respectively. The direction of moment is not known. Moreover, at 41 K the magnetic susceptibility undergoes a sudden change, whose nature is not fully understood [1]. Despite the large U-U distance (d = 4.24 Å) numerous findings suggest that the antiferromagnetism of UGa_3 is itinerant: I) the small ordered moment of 0.6 – 0.8 μ_B in the ordered state, II) the lack of any Curie-Weiss like behaviour in the paramagnetic susceptibility, III) the small cusp-like anomaly in the resistivity at T_N [2].

Previous dHvA measurements claimed a fair agreement with calculations in local density approximation (LDA), where the 5f electrons are treated as ordinary band electrons (i.e. itinerant) [3]. However, more recent and complete dHvA experiments [4] show that they can not be fully explained by standard LDA calculations with f-electrons treated either as itinerant or localized (open-core treatment, OC).

We measured the 2-dimensional angular correlation of the positron annihilation radiation (2D-ACAR) of UGa_3 in the paramagnetic phase, for five crystal orientations. As a result of the momentum conservation of the annihilated particles, 2D-ACAR spectra provide 2D projections of the electron-positron momentum density $\rho^{ep}(\boldsymbol{p})$. The application of the Lock Crisp West transformation (LCW) [5] to $\rho^{ep}(\boldsymbol{p})$ yields then a projection of the Fermi volume in the first Brillouin zone (BZ). Figure 1 shows the projections of the LCW k-space densities along the [001] crystal axes of UGa_3 and the isostructural 4f electron systems $TmGa_3$ and $ErGa_3$, where the localization of the 4f electrons was proved by dHvA and 2D-ACAR experiments [6,7]. Interestingly, in spite of some similarity at the corners of the projected BZ (MR points) noticeable differences appear throughout the BZ.

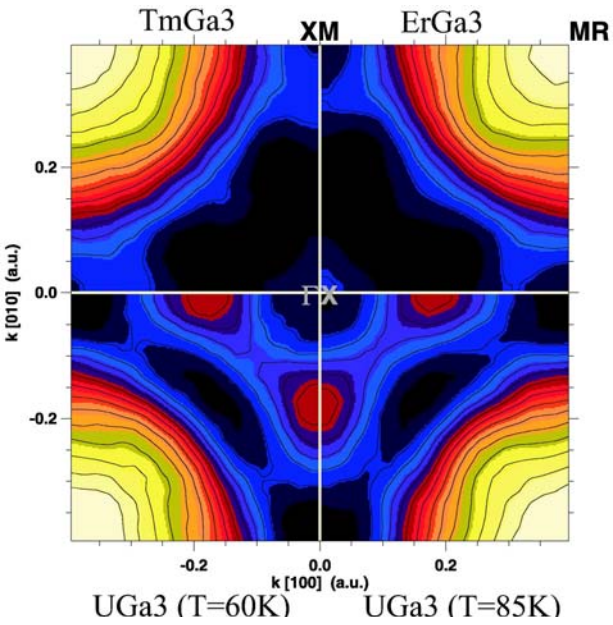

Figure 1: Projections of $\rho^{LCW}(\boldsymbol{k})$ distributions in UGa_3 for two different temperatures and corresponding projections from two isostructural compounds $TmGa_3$ and $ErGa_3$

To complement our experimental results, we performed set of calculations in the framework of density functional theory (DFT) with LDA treatment of exchange-correlation effects using full-potential augmented plane waves method implemented in WIEN2k [8]. To test itinerancy of 4f electrons we performed standard band calculation, OC calculation and three calculations, where we treated 1, 2

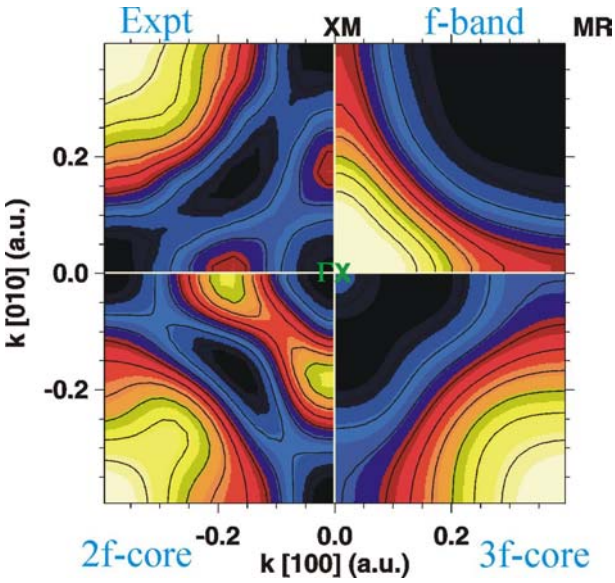

Figure 2: Projections of experimental (left top) and calculated Fermi surfaces of UGa_3. Top right displays results for 5f in band calculation, bottom right is from standard open-core calculation and bottom left corresponds to calculations with two 5f electrons treated as localized core states

and 3 5f-electrons as core electrons (i.e. localized) while allowing band 5f states to be occupied.

The experimental results are in clear discrepancy with the results of density functional calculations (DFT) with 5f electrons treated as itinerant. Results of OC calculations show slightly better agreement, but still not satisfactory. A relevant improvement is obtained by constraining only 2 f-electrons to be part of the core. With this constraint we obtained occupancy of band 5f states 0.7, so the f-electrons will contribute to the Fermi surface. We calculated the same Fermi surface projections as obtained from experiment and displayed our results on Figure 2. These calculations strongly support a dual character of f-electrons in this system.

We must note, that this kind of calculations in WIEN2k leads to wave functions of different 5f states (core and band states), which are not completely orthogonal. Effect of this error has to be investigated.

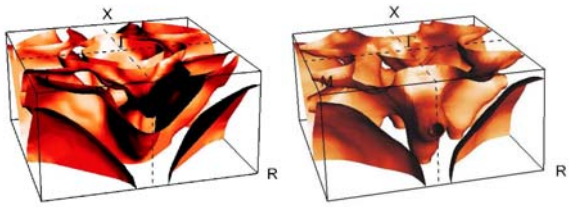

Figure 3: Calculated (left) and experimental reconstructed (right) Fermi surfaces for UGa_3

Finally, by making use of the five collected projections of $\rho^{ep}(\boldsymbol{p})$ in UGa_3 and adopting tomographic reconstruction techniques we produced the 3D k-space density $\rho^{LCW}(\boldsymbol{k})$ and, consequently, the Fermi surface. It is worth noting that the resolution of our experiment (equivalent to an average 13% of the linear size of the BZ) allows only limited reconstruction of Fermi surface. In this case, calculations lead to a very complicated topology (despite the fact, that there is only one band crossing Femi level), which could not be obtained in full detail taking into account the experimental resolution. Thus, comparison of theoretical and experimental Fermi surface topology can be only approximate. Bearing this in mind, obtained plots of Fermi surface topology show important similarities.

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